chain nodes :
    21 22 23 24 25 26 27 28 29 30 31 32 34 35 36 37 39 41 42
ring nodes :
    1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
chain bonds :
    1-42 2-41 6-22 8-27 10-21 14-28 15-19 16-24 16-31 17-25 17-32 19-29 20-23 20-30
    21-22 25-26 34-35 35-36 35-37
ring bonds :
    1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 11-13 12-15 13-14 14-15
    16-17 16-20 17-18 18-19 19-20
exact/norm bonds :
    10-21 11-13 12-15 13-14 14-15 15-19 16-17 16-20 16-24 17-18 18-19 19-20 20-23
    34-35 35-36
exact bonds :
    1-42 2-41 6-22 8-27 14-28 16-31 17-25 17-32 19-29 20-30 21-22 25-26 35-37
normalized bonds :
    1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

G1:I,SO3H,C(O)CH3,[*1]

Match level :
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
    12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:CLASS
    22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
    31:CLASS 32:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS 39:CLASS 40:Atom 41:CLASS
    42:CLASS